Strain-dependence of the superconducting critical temperature $T_c$ in Al and Nb simple crystals from first-principles M. SALVETTI, N. BONINI, M.I.T., M. CALANDRA, IMPMC/CNRS, D. PARKS, N. MARZARI, J. MINERVINI, M.I.T. — In the past 20 years, efforts have been devoted to predict the critical current density $J_c$ of superconducting magnets based on the Nb$_3$Sn compound. The use of Nb$_3$Sn magnets for high-field applications has highlighted the dependence of $J_c$ on strain. We present calculations of the $T_c$-dependence of Al and Nb crystals on pressure, uni-axial and shear strains using the DFT PWscf package from the Quantum-ESPRESSO distribution to evaluate the phonon linewidth and the $el-ph$ coupling parameter using very dense $k$-space samplings of the IBZ. The superconducting critical $T_c$ is calculated by using the McMillan formula as a fit to the solution of the Migdal-Eliashberg equations. Favourable comparisons with available experimental data have been obtained and will be presented. The modelling of the $T_c$-dependence on strain in Nb$_3$Sn crystals is an ongoing effort. The potential for modelling the $T_c$-dependence on strain in Nb$_3$Sn is discussed. In this regard, recent advances in the implementation of the Wannier formalism give access to the sampling of the dense $k$-point grids required to calculate fully-converged electron-phonon coupling quantities. This approach opens the possibility to extend the study of the $T_c$-dependence on strain to unit cells characterized by a higher number of atoms or electronic complexity.

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Date submitted: 21 Nov 2008

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